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Local Sensitivity of Predicted CO₂ Injectivity and Plume Extent to Model Inputs for the FutureGen 2.0 site

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Abstract

Numerical simulations have been used for estimating CO₂ injectivity, CO₂ plume extent, pressure distribution, and Area of Review (AoR), and for the design of CO₂ injection operations and monitoring network for the FutureGen project. The simulation results are affected by uncertainties associated with numerous input parameters, the conceptual model, initial and boundary conditions, and factors related to injection operations. Furthermore, the uncertainties in the simulation results also vary in space and time. The key need is to identify those uncertainties that critically impact the simulation results and quantify their impacts. We introduce an approach to determine the local sensitivity coefficient (LSC), defined as the response of the output in percent, to rank the importance of model inputs on outputs. The uncertainty of an input with higher sensitivity has larger impacts on the output. The LSC is scalable by the error of an input parameter. The composite sensitivity of an output to a subset of inputs can be calculated by summing the individual LSC values.

We propose a local sensitivity coefficient method and applied it to the FutureGen 2.0 Site in Morgan County, Illinois, USA, to investigate the sensitivity of input parameters and initial conditions. The conceptual model for the site consists of 31 layers, each of which has a unique set of input parameters. The sensitivity of 11 parameters for each layer and 7 inputs as initial conditions is then investigated. For CO₂ injectivity and plume size, about half of the uncertainty is due to only 4 or 5 of the 348 inputs and 3/4 of the uncertainty is due to about 15 of the inputs. The initial conditions and the properties of the injection layer and its neighbour layers contribute to most of the sensitivity. Overall, the simulation outputs are very sensitive to only a small fraction of the inputs. However, the parameters that are important for controlling CO₂ injectivity are not the same as those controlling the plume size. The three most sensitive inputs for injectivity were the horizontal permeability of Mt Simon 11 (the injection layer), the initial fracture-pressure gradient, and the residual aqueous saturation of Mt Simon 11, while those for the plume area were the initial salt concentration, the initial pressure, and the initial fracture-pressure gradient. The advantages of requiring only a single set of simulation results, scalability to the proper parameter errors, and easy calculation of the composite sensitivities make this approach very cost-effective for estimating AoR uncertainty and guiding cost-effective site characterization, injection well design, and monitoring network design for CO₂ storage projects.

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1. Introduction

Although the uncertainty of model inputs directly affects the accuracy of numerical simulation of CO₂ migration in the reservoir, model predictions often are more sensitive to some inputs than others. Sensitivity analysis is a powerful tool in ranking the importance of model inputs on the predictions of a model.

The methods for sensitivity analysis can be generally divided into two categories, one for the global sensitivity and the other for the local sensitivity. The global method using Monte Carlo simulations is often used to determine the prediction uncertainty, by quantifying and propagating uncertainty in major input parameters. Reliable uncertainty analysis generally requires a large number of realizations (e.g., 100s or more for several parameters) for statistically stable results, and this number increases exponentially with the number of parameters to be investigated [1,2]. Simulation of field-scale CO₂ injection at the injection rate of about 1.1 MMT/yr for decades generally requires a very large three-dimensional domain (e.g., 10s to 100s of km in the horizontal directions), fine enough discretization to correctly predict plume size and shape, and small enough time steps to accurately simulate non-uniform injection due to power plant and well maintenance. Therefore, the simulation is often computationally intensive, e.g., taking days or weeks or even longer to complete. As a result, investigating the impacts of hundreds of model inputs using the Monte Carlo approach can be computationally impractical in many cases [1-4].

The local sensitivity approach involves taking the partial derivative of the output with respect to an input factor at a fixed local point. For numerical models, the partial derivative can be approximated by a difference quotient. The approach is to vary one input at a time relative to a reference case, giving rise to the local sensitivity to each of the input parameters. The local sensitivity approach is accurate if the response of the output to an input is linear. Otherwise, the local sensitivity may not represent the sensitivity in the overall parameter space. In spite of this limitation, the local sensitivity analysis is still advantageous for ranking the importance of model inputs. Some researchers [5] argued that many models of natural systems are linear enough for local sensitivity analysis to be useful; the local and global methods can provide consistent results in ranking the importance of inputs [6]. The local sensitivity approach has been used to investigate pressure response to input parameters for CO₂ storage projects [7]. One advantage of the local sensitivity approach is that the number of simulations needed to be performed is linearly, rather than exponentially as in the Monte Carlo approach, proportional to the number of the model inputs to be investigated. Hence, the local sensitivity analysis approach can possibly be used to investigate the sensitivity of a prediction to a very large number of parameters [6,7].

The purpose of this study is to propose a method to calculate the local sensitivity coefficient and apply it to the FutureGen 2.0 Site in Morgan County, Illinois, USA [8,9], to rank the importance of input parameters to plume size and CO₂ injectivity. The CO₂ injectivity is defined as the total mass of CO₂ injected into the injection zone.

Nomenclature

b	fraction change in a log-normally distributed variable
i	index of an input
C_i	local sensitivity coefficient
C_i^S	scaled local sensitivity coefficient
C^S	composite scaled local sensitivity coefficient for a subset or all of the inputs
C_{ab}^S	absolute composite scaled local sensitivity coefficient for a subset or all of the inputs

M	number of a subset of inputs
N	number of total inputs
X	model inputs
Y	model output
Y_0	model output of the reference case
Y_i	model output when the i^{th} input is varied
σ	standard deviation
ΔX	change in input X from the reference case

2. Local Sensitivity Coefficient

In numerical simulation of CO₂ injection, the output, Y, such as plume extent or CO₂ injectivity is a function of N inputs (i.e., X₁ through X_N). Namely,

$$Y_0 = f(X_1, X_2, \dots, X_i, \dots, X_N) \quad (1)$$

For numerical models, the response of output Y to the change of an input X_i is calculated by varying the input by a small amount, ΔX_i :

$$\Delta Y_i = Y_i - Y_0 = f(X_1, X_2, \dots, X_i + \Delta X_i, \dots, X_N) - f(X_1, X_2, \dots, X_i, \dots, X_N) \quad (2)$$

There are many ways to quantify the local sensitivity [5,6]. The local sensitivity coefficient (LSC) for each of the inputs, C_i, here is defined here as the response of the output in percent:

$$C_i = 100\Delta Y_i / Y_0 = 100(Y_i / Y_0 - 1) \quad (3)$$

A greater-than-zero value of C_i means a positive impact of input X_i on output Y and, vice versa, a less-than-zero value means a negative impact. Hence, an input has the largest sensitivity when the absolute value of C_i is the largest. This definition of local sensitivity coefficient is simpler than those in [5] or [6] because no weighting factors are needed. It will take only N+1 simulations to compute C_i for each of the N model inputs.

To calculate C_i(%) for each of the inputs, the change in each input, ΔX_i , must be determined before the simulation can be executed. In order to make the comparison meaningful, ΔX_i should reflect the uncertainty of the input X_i. It is recommended that the standard deviation, σ_{xi} , of X_i be used if X_i is normally distributed (ND) or the standard deviation, $\sigma_{\ln xi}$, of $\ln(X_i)$ be used if X_i is log-normally distributed (LND). However, often times the σ_{xi} or $\sigma_{\ln xi}$ values are not known beforehand. In this case, an initial best guess can be used for the simulations. A good approximation is the measurement error of X_i. ΔX_i will be a constant for ND inputs (e.g., porosity) and a fraction of X_i (i.e., $\Delta X_i = bX_i$, where b is a constant) for LND inputs (e.g., permeability).

With the linear assumption, the local sensitivity can be rescaled to estimate the response of predictions at a different value of parameter uncertainty based on the completed simulations. Hence there is no need to rerun the simulation if the uncertainty value is different from the value used in the already completed simulations. However, if the impact of a parameter is nonlinear, the accuracy of the estimated sensitivity decreases when the difference between the new and old uncertainty values increases. Then, after the simulation, the scaled local sensitivity coefficient, C_i^S, can be estimated using known σ_{xi} or $\sigma_{\ln xi}$:

$$C_i^S = \begin{cases} C_i \frac{\sigma_{xi}}{\Delta X_i} & \text{for ND inputs} \\ C_i \frac{\sigma_{\ln xi}}{\ln(1+b_i)} & \text{for LND inputs} \end{cases} \quad (4)$$

Based on the first-order approximation of the Taylor series over multiple variables, the local sensitivities to different parameters are additive, assuming that parameters are independent of one another in the model. This assumption requires that the value of an input not be calculated based on one or more of the other inputs. For example, porosity and permeability often have a good correlation. In this case, if permeability is calculated based on porosity, they are not independent. Otherwise, if they are determined separately, they are still independent inputs. This means that, based on the simulation results of the sensitivity to individual inputs, the composite sensitivity of a prediction to a subset of M ($M \leq N$) inputs can be readily calculated by summing up the individual C_i^S values:

$$C^S = \sum_1^M C_i^S \quad (5)$$

The subset of inputs can be the same or different type of inputs. Because ΔX_i and b can be either positive or negative, Eq. (5) may only be used if the signs (positive or negative) of ΔX_i and b are known because positive and negative C_i^S values cancel each other. The absolute composite scaled sensitivity coefficient, which is the maximum sensitivity for the subset or all of inputs, is the sum of the absolute values of C_i^S :

$$C_{ab}^S = \sum_1^M |C_i^S| \quad (6)$$

3. Materials and Methods

We applied the local sensitivity approach to the FutureGen 2.0 Site in Morgan County, Illinois, USA [8,9], to investigate the sensitivity of CO_2 injectivity and plume size to input parameters and initial conditions.

3.1. The STOMP Simulator

The simulations conducted for this investigation were executed using the STOMP- CO_2 simulator [10-12]. Partial differential conservation equations for the aqueous fluid mass, separate-phase CO_2 mass, energy, and salt mass compose the fundamental equations for STOMP- CO_2 . A fully coupled well model is defined in STOMP- CO_2 as a source that extends over multiple grid cells to simulate the injection of CO_2 under a specified mass injection rate, subject to a pressure limit [13]. The CO_2 injection rate is proportional to the pressure gradient between the well and surrounding formation in each grid cell.

For the range of temperature and pressure conditions present in deep saline reservoirs, four phases are possible: 1) water-rich liquid, 2) CO_2 -rich gas, 3) CO_2 -rich liquid (liquid CO_2), and 4) precipitated salt. The equations of state express the existence of phases given the temperature, pressure; water, CO_2 , and salt concentration; the partitioning of components among existing phases; and the density of the existing phases. Physical processes modeled in the simulations included isothermal multi-fluid flow and transport for three components (i.e., water, salt, and CO_2) and two phases (i.e., aqueous and CO_2 rich phase).

3.2. Conceptual Model and CO_2 Injection

A stratigraphic conceptual model of the geologic layers from the Precambrian basement to the secondary confining zone was constructed using the EarthVision® software package. The geological units from top to bottom

included the Franconia, Ironton, Eau Claire (Proviso, Lombard, and Elmhurst), Mount Simon, and Precambrian formations [8]. There is a regional dip of approximately 0.25 degree in the east-southeast direction. The conceptual model was expanded to a lateral domain size of 100- by 100-mi for numerical simulation and was further divided into 31 simulation layers (Table 1), each of which has a unique set of input parameters. The three-dimensional, boundary-fitted numerical model grid was designed to have constant grid spacing with higher resolution in the area influenced by the CO₂ injection (3- by 3-mi area), with increasingly larger grid spacing moving out in all lateral directions toward the domain boundary. The 3-dimensional domain is discretized into $60 \times 60 \times 31 = 111600$ elements.

The system was assumed to be at steady state until the start of injection. The bottom boundary was set as a no-flow boundary for all the fluids and components. The lateral and top boundary conditions were set to hydrostatic pressure with the assumption that each of these boundaries is distant enough from the injection zone. The CO₂ is primarily injected into the layer named MtSimon11 for 20 years in four lateral injection wells, whose lengths range between 1500 ft and 2500 ft. It was assumed that there were 5 planned well maintenance episodes with a total length of 72.875 days every 1.5 years and this cycle continued for 20 yrs. The injection rate was pressure controlled during the injection period and zero when the system was under maintenance. For the reference case, the average total injection rate for the 4 wells was about 1.1 MMT/yr.

Table 1. Division of Stratigraphic Layers into Computational Model Layers

Formation	Layer Name	Top Depth (ft KB [#])	Top Elevation (ft)	Bottom Elevation (ft)	Thickness (ft)	Layer Number	Zone
Franconia	Franconia	3086	-2453	-2625	172	31	Secondary Confining Zone
Davis-Ironton	Davis-Ironton	3258	-2625	-2697	72	30	
Ironton-Galesville	Ironton-Galesville	3330	-2697	-2806	109	29	
Proviso	Proviso4_5	3439	-2806	-2891	85	28	Primary Confining Zone
	Proviso1_3	3524	-2891	-2963	72	27	
Lombard	Lombard12_14	3596	-2963	-3073	110	26	
	Lombard8_11	3706	-3073	-3137.5	64.5	25	
	Lombard5_7	3770.5	-3137.5	-3161	23.5	24	Injection Zone
	Lombard1_4	3794	-3161	-3219	58	23	
Elmhurst	Elmhurst7	3852	-3219	-3229	10	22	
	Elmhurst6	3862	-3229	-3239	10	21	
	Elmhurst5	3872	-3239	-3249	10	20	
	Elmhurst4	3882	-3249	-3263	14	19	
	Elmhurst3	3896	-3263	-3267	4	18	
	Elmhurst2	3900	-3267	-3277	10	17	
	Elmhurst1	3910	-3277	-3289	12	16	
Mount Simon	MtSimon17	3922	-3289	-3315	26	15	
	MtSimon16	3948	-3315	-3322	7	14	
	MtSimon15	3955	-3322	-3335	13	13	
	MtSimon14	3968	-3335	-3355	20	12	
	MtSimon13	3988	-3355	-3383	28	11	
	MtSimon12	4016	-3383	-3404	21	10	
	MtSimon11	4037	-3404	-3427	23	9	
	MtSimon10	4060	-3427	-3449	22	8	
	MtSimon9	4082	-3449	-3471	22	7	
	MtSimon8	4104	-3471	-3495	24	6	
	MtSimon7	4128	-3495	-3518	23	5	
	MtSimon6	4151	-3518	-3549	31	4	
	MtSimon4_5	4182	-3549	-3627	78	3	
	MtSimon2_3	4260	-3627	-3717	90	2	
	MtSimon1	4350	-3717	-3799	82	1	

[#]Kelly Bushing (KB) is 14 ft above ground surface

3.3. Sensitivity Analysis

The sensitivities to 11 parameters for each of the 31 layers were investigated relative to a reference case, which was the most representative case based on the characterization data available [14]. The parameters, changes in parameter values, and the assumed standard deviation are summarized in Table 2. These parameters describe the physical properties of the rocks. In total there were 341 ($= 31 \times 11$) parameters evaluated. Additionally, the sensitivities to 7 inputs that describe the initial conditions of the simulation were examined (Table 3). The standard deviation for each of the inputs presented in this paper was assumed for the purpose of demonstration. The actual values may be different.

There were 349 simulations performed in total for 348 inputs. These simulations were executed using PNNL Institutional Computing at Pacific Northwest National Laboratory. After the completion of the simulations, the injectivity of CO₂ and the plume area was calculated for each simulation at different times.

Table 2. Changes in Parameter Values and the Assumed Standard Deviation for Sensitivity Analysis

	Name	Parameter Symbol	Units	Ln-Transformed?	ΔX or b^*	Assumed σ_x
1	Porosity	por	m ³ m ⁻³	No	0.01	0.01
2	Horizontal Permeability	kh	mD	Yes	0.1	0.095
3	Vertical Permeability	kv	mD	Yes	0.1	0.095
4	Gas Entry Pressure	pe	m	Yes	0.1	0.095
5	Pore Size Distribution Parameter Lambda	lambda	-	No	0.1	0.1
6	Residual Water Content	srw	-	No	0.1	0.1
7	Maximum Trapped Gas Content	srn	-	No	0.1	0.1
8	Grain Density	rho_g	kg m ⁻³	No	100	100
9	Pore Compressibility	comp	pa ⁻¹	Yes	0.1	0.095
10	Thermal Conductivity	kt	W m ⁻¹ K ⁻¹	Yes	0.1	0.095
11	Heat Capacity	cp	J kg ⁻¹ K ⁻¹	No	100	100

*b for the ln-transformed variables and ΔX for other variables

Table 3. Changes in Initial Conditions and the Assumed Standard Deviation for Sensitivity Analysis

	Name	Parameter Symbol	Units	Ln-Transformed?	ΔX	Assumed σ_x
1	Salt Fraction	c	-	No	0.01	0.01
2	Salinity Gradient	cg	ft ⁻¹	No	0.00001	0.00001
3	Injection Zone Pressure	p	psi	No	10	10
4	Temperature	t	°F	No	10	2
5	Temperature Gradient	tg	°F ft ⁻¹	No	0.001	0.001
6	Fracture-Pressure Gradient	fg	psi ft ⁻¹	No	0.065	0.065
7	Injection Temperature	t	°F	No	5	5

4. Results

After the simulations were completed, the sensitivity coefficients of CO₂ injectivity and plume area to each of the 348 inputs were calculated using Eqs. (3) and (4) for different times. The absolute composite sensitivity coefficients were then calculated using Eq. (6) for the 11 parameters and the initial conditions and for each of the 31 layers. The results reported here are for the injectivity and plume area at 20 yrs, the time at which injection ceased.

4.1. CO₂ Injectivity

With the assumed uncertainties in inputs (Tables 2 and 3), there is an overall absolute composite sensitivity of 31.6% on the injectivity, meaning that, in the worst case scenario (no cancellation of impacts on output), the uncertainty in CO₂ injectivity is 31.6%. The local sensitivity coefficients for the top 15 most sensitive inputs are shown in Fig. 1. Among the 348 inputs, about 1/2 of the uncertainty in CO₂ injectivity was attributed to the top 4

inputs, i.e., horizontal permeability of the injection layer (MtSimon11), fracture-pressure gradient, residual saturation of the injection layer, and initial pressure of the system. About $\frac{3}{4}$ of the uncertainty was due to the top 15 inputs.

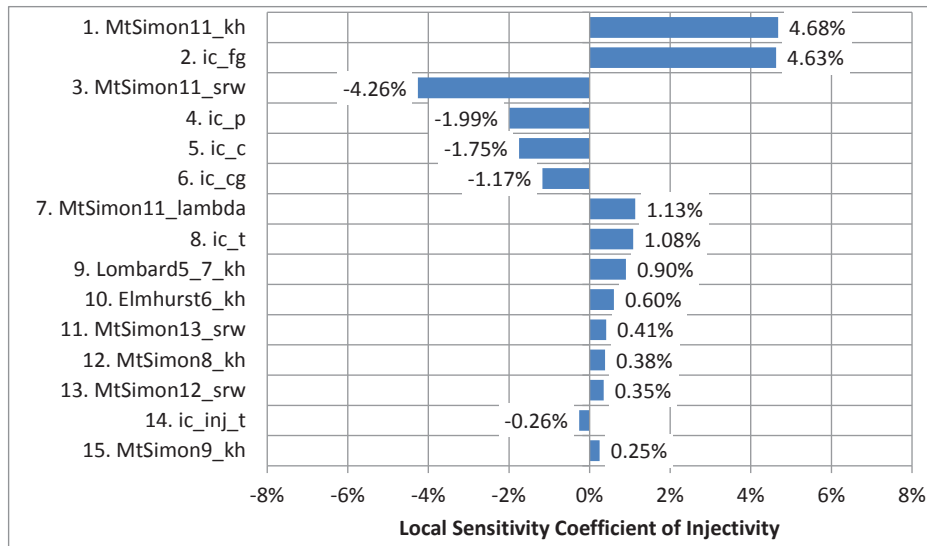


Fig. 1. The local sensitivity coefficient of CO₂ injectivity to the top 15 most sensitive inputs. The numbers in the plot represent the percent of injectivity relative to that of the reference case. The labels in the vertical axis are the combination of the following: rank of the input, rock layer name listed in Table 1 or initial condition (ic), and the name of the inputs listed in Tables 2 or 3.

The absolute composite sensitivities to input types (Fig. 2a) indicate that three input types, i.e., the initial conditions, horizontal permeability, and residual aqueous saturation, cause more than $\frac{3}{4}$ of the uncertainty for injectivity. The absolute composite sensitivities for rock layers (initial conditions were excluded) indicate that nearly half of the uncertainty in injectivity was due to the properties of the MtSimon11, which is the injection layer. Among the rest of the layers, the injectivity is relatively more sensitive to the properties of the layers in the injection zone (from MtSimon1 to Lombard1_4, Table 1) than those in the confining zone.

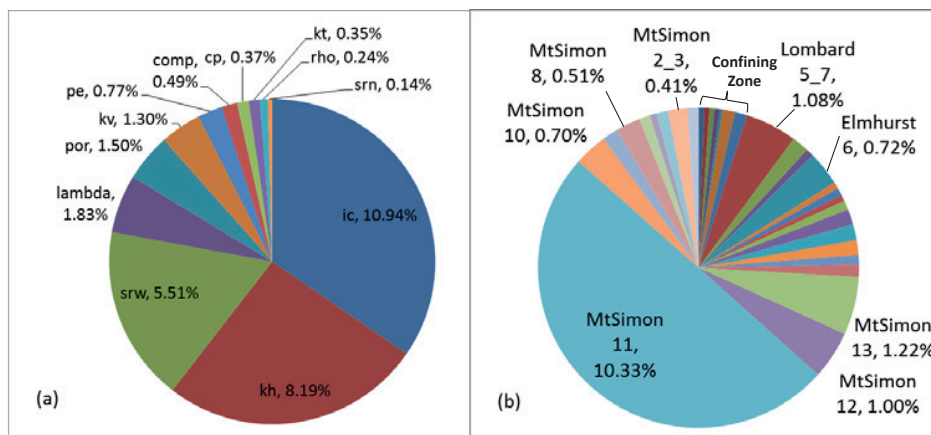


Fig. 2. (a) The absolute composite sensitivity coefficient of CO₂ injectivity to the 12 input types. (b) The absolute composite sensitivity coefficient of CO₂ injectivity to the 31 layers. The numbers in the plot represent the percent of injectivity relative to that of the reference case. In plot (a), ic stands for initial condition and other symbols are listed in Table 2. In plot (b), the names of the rock layers (see Table 1) and the absolute composite sensitivity coefficients are shown for only a few most sensitive layers.

4.2. CO₂ Plume Area

Because the total CO₂ mass injected was different among the simulation cases, for a fair comparison, the plume area was scaled as if the mass injected had been the same as that of the reference case. With the assumed uncertainties in inputs (Tables 2 and 3), there is an overall absolute composite sensitivity of 42.7% on the plume area, meaning that, in the worst case scenario (no cancellation of impacts on output), the uncertainty in plume area is 42.7%. The local sensitivity coefficients for the top 15 most sensitive inputs are shown in Fig. 3. About half of the uncertainty in plume area was due to the top five inputs. About ¾ of the uncertainty in plume area was due to the 15 of the inputs.

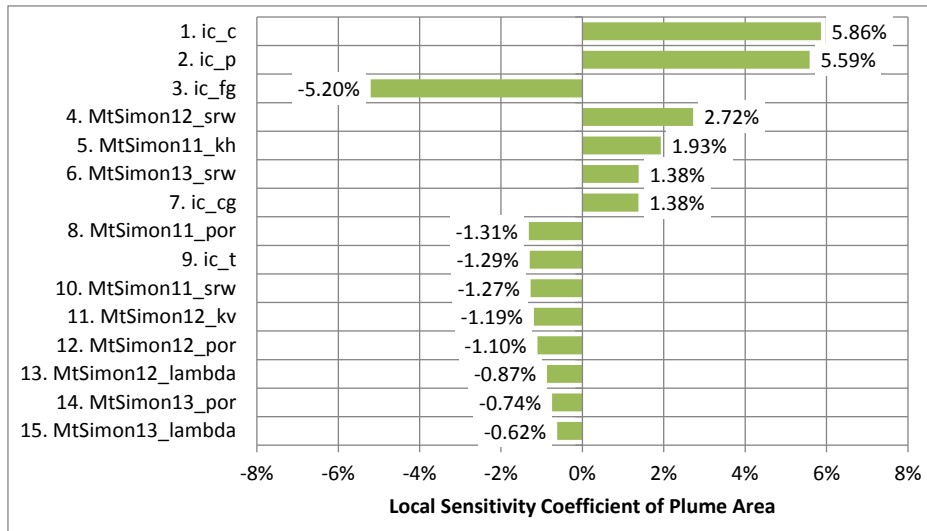


Fig. 3. The local sensitivity coefficient of CO₂ plume area to the top 15 most sensitive inputs. The numbers in the plot represent the percent of plume area relative to the reference case. The labels in the vertical axis are the combination of the following: rank of the input, rock layer name listed in Table 1 or initial condition (ic), and the name of the inputs listed in Tables 2 or 3.

The absolute composite sensitivities of plume area to the 12 types of inputs are shown in Fig. 4a. The initial conditions result in nearly half of the uncertainty in plume area, while the residual aqueous saturation and horizontal permeability result in about ¼ of the uncertainty, and the rest of the inputs contribute to the rest ¼ uncertainty. The absolute composite sensitivities to the properties of the 31 layers (initial conditions were excluded) are shown in Fig. 4b. The properties of MtSimon 11, 12 and 13 contribute to about 2/3 of the sensitivity. As expected, the properties of the confining zone have little impact on the plume area.

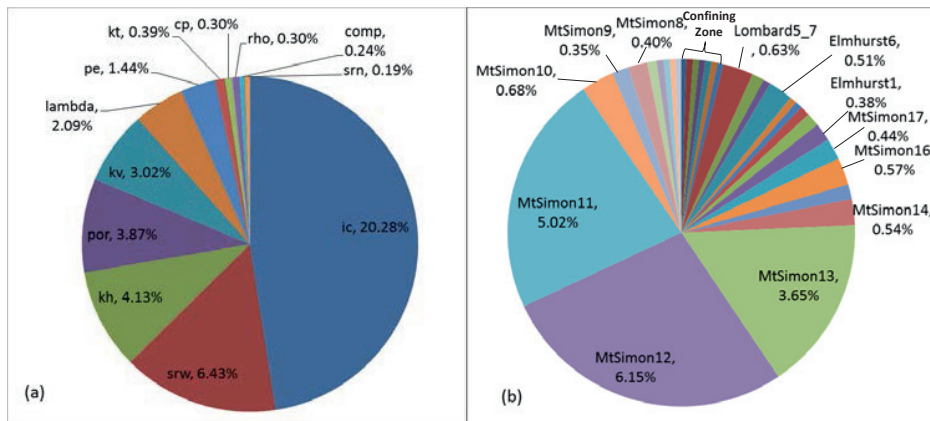


Fig. 4. (a) The absolute composite sensitivity coefficient of CO₂ plume area to the 12 input types. (b) The absolute composite sensitivity coefficient of CO₂ plume area to the 31 layers. The numbers in the plot represent the percent of plume area relative to the reference case. In plot (a), ic stands for initial condition and other symbols are listed in Table 2. In plot (b), the names of the rock layers (see Table 1) and the absolute composite sensitivity coefficients are shown for only a few most sensitive layers.

5. Summary

The local-sensitivity approach is capable of efficiently identifying the inputs that most influence the model prediction of CO₂ injectivity and plume size, particularly when the total number of inputs is large (e.g., 10s or 100s), and the use of a global approach is impractical. This approach is useful for ranking model inputs, and these results will be useful for AoR uncertainty estimation, cost-effective site characterization, injection well design, and monitoring network design. We proposed a method to calculate the local sensitivity coefficient that is defined as the response of the output in percent to the change of an input. According to the first-order expansion of the Taylor series over multiple variables, the local sensitivity coefficients for different parameters are additive so that the composite sensitivity of a certain input or of a sub-zone can be calculated, assuming that the parameters are independent of one another in the model. They can also be rescaled to estimate the uncertainty of predictions for an uncertainty value that is different from those listed in Tables 2 and 3, removing the need to rerun the simulation.

Application of this approach to the FutureGen 2.0 Site in Morgan County, Illinois, USA shows that the sensitivity of CO₂ injectivity to model inputs varied significantly. Among the 348 inputs, half of the uncertainty in CO₂ injectivity and CO₂ plume extent was attributed to the most sensitive 4 or 5 inputs and about $\frac{3}{4}$ of the uncertainty was attributed to about 15 inputs. The initial conditions and the properties of the injection layer and its neighbor layers contribute to most of the sensitivity. This suggests that, during site characterization, more effort should be directed at better quantifying the most sensitive parameters. However, the results indicate that the parameters that are important for controlling CO₂ injectivity are not the same as those for controlling the plume size. The three most sensitive inputs for injectivity were the horizontal permeability of Mt Simon 11 (the injection layer), the initial fracture-pressure gradient, and the residual aqueous saturation of Mt Simon 11, while those for the plume area were the initial salt concentration, the initial pressure, and the initial fracture-pressure gradient. Therefore, it is important for CO₂ storage projects to determine priorities and plan their site characterization efforts accordingly. The approach presented here can be used for determining the sensitivity for other outputs (e.g., pressure in the confining zone), other times (e.g., 5, 10, or 15 yr), or other locations (e.g., monitoring locations), to determine which model parameters are sensitive to selected outcomes.

The local sensitivity analysis approach can be a very useful tool for evaluating the importance of numerical model inputs relative to a reference case. For evaluating the sensitivity over the entire parameter space, it is more appropriate to use global sensitivity methods such as the Monte Carlo approach with a selected list of model inputs.

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